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A METHOD FOR APPROXIMATING EQUIVALENT CORROSION TIME FROM EXPERIMENTAL DATA

TMI-1863

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In many developmental tests it is necessary to operate at conditions which are somewhat transient; that is, material and gas temperatures vary with time. Corrosion analysis of these tests is, therefore, difficult to analyze because corrosion rate is an exponential function of temperature.

A fortran program was written to determine the equivalent corrosion time at a particular temperature based on the experimental temperature-time curve.

The reaction rate of carbon removal is approximated by the following expression:

$$\frac{dm}{dt} = \pi \left\{ k_1 \left[Y_{H_2} - \frac{1}{K_{p_1} \pi} \frac{Y_{CH_4}}{Y_{H_2}} \right] + k_3 \left[Y_{H_2} - \frac{1}{K_{p_2}} Y_{C_2H_2} \right] \right\}$$

where

m = mass (lb.)

t = time

Y_i = weight fraction of gas, i, in the gas stream

K_{p_1} = equilibrium constants, atm^{-1}

π = total pressure, atm.

For the case in which a fresh stream of hydrogen is available to an uncoated graphite surface and the concentration of hydrocarbons in the gas stream and at the graphite surface is small, it can be assumed that,

$$Y_{H_2} = 1 \qquad Y_{CH_4} = Y_{C_2H_2} = 0$$

The equation then reduces to:

$$\frac{dm}{dt} = \pi \; (k_1 + k_3)$$

In general

$$k_1 = A_1 \, e^{-B_1/T} \qquad \text{lb Carbon/in}^2\text{-sec-atm.}$$

$$k_3 = A_3 \, e^{-B_3/T} \qquad \text{lb Carbon/in}^2\text{-sec-atm.}$$

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where

A_1 and B_1 are reaction rate constants for methane formation,

A_3 and B_3 are reaction rate constants for acetylene formation, and

T is the absolute temperature.

The amount of carbon/area removed during a test of duration $t = 0$ to $t = t_1$ would be:

$$Mo - M = \int_{Mo}^{M} dm = \pi \int_{0}^{t_1} \left(A_1 e^{-B_1/T} + A_3 e^{-B_3/T} \right) dt$$

where

$$T = f(t)$$

If the independent variable, t, is changed to the dimensionless variable

$$\eta = t/t_1$$

the mass removal would be rewritten:

$$Mo - M = \pi t_1 \int_{0}^{1} \left(A_1 e^{-B_1/T} + A_3 e^{-B_3/T} \right) d\eta$$

where

$$T = f(\eta \times t_1)$$

For a constant temperature, Tr, the amount of carbon removed during a given time period $t = 0$ to $t = t_r$ would be:

$$Mo - M = \pi t_r \int_{0}^{1} \left(A_1 e^{-B_1/Tr} + A_3 e^{-B_3/Tr} \right) d\eta$$

$$= \pi t_r \left(A_1 e^{-B_1/Tr} + A_3 e^{-B_3/Tr} \right)$$

For equivalent mass removal at both the reference temperature and the experimental temperature curve, equate the two mass removal expressions:

$$\pi t_r\left(A_1 e^{-B_1/Tr} + A_3 e^{-B_3/Tr}\right) = \pi t_1 \int_0^1 \left(A_1 e^{-B_1/T} + A_3 e^{-B_3/T}\right) d\eta$$

$$t_r = t_1 \frac{\int_0^1 \left(A_1 e^{-B_1/T} + A_3 e^{-B_3/T}\right) d\eta}{A_1 e^{-B_1/Tr} + A_3 e^{-B_3/Tr}}$$

Let

$$C = A_1 e^{-B_1/Tr} + A_3 e^{-B_3/Tr}$$

$$Z = \int_0^1 \left(A_1 e^{-B_1/T} + A_3 e^{-B_3/T}\right) d\eta$$

Solving the integral by use of Simpson's rule (Parabolic Rule) for an even number of spaces (n) in the interval of $\eta = 0$ to $\eta = 1$ produces the following form.

If

$$X_i = A_1 e^{-B_1/T_i} \qquad i = 0, n$$

$$Y_i = A_3 e^{-B_3/T_i} \qquad i = 0, n$$

Then

$$Z = \Big[(Xo + 4X_1 + 2X_2 + 4X_3 + \ldots . + 2X_{n-2} + 4X_{n-1} + X_n) + (Yo + 4Y_1 + 2Y_2 + 4Y_3 + \ldots . + 2Y_{n-2} + 4Y_{n-1} + Y_n)\Big] /3n$$

Where

n = Number of time intervals the time-temperature curve is broken up into (even number).

T_o, T_1, ... T_n = the temperature at equal time intervals (odd number of T_i's) throughout the test.

Therefore,

$$t_r = t_1 \frac{Z}{C}$$

FORTRAN PROGRAM

This program was written for the CDC 6600 computer and is designed to take experimental time-temperature profiles and equate the corrosion to a specific reference temperature and calculate an equivalent corrosion time. The program is set to calculate the equivalent corrosion time for several different reference temperatures, varying from TRO to TRF in steps of TRS. i.e. The reference temperatures would be

TRO, TRO + TRS, TRO + 2xTRS, ..., TRO + NxTRS

where

(TRO + NxTRS) = TRF

DESCRIPTION OF INPUT DATA

1. Experimental temperature readings must be taken at equal time intervals where the number of temperature readings, R, must be odd.
2. The first data card contains the following reaction rate constants:

A_1	= constant associated with methane formation rate.	Col. 1-12
B_1	= constant associated with the exponential term of the methane formation rate (positive value) (^oR).	Col. 13-24
A_3	= constant associated with acetylene formation rate.	Col. 25-36
B_3	= constant associated with the exponential term of the acetylene formation rate (positive value) (^oR).	Col. 37-48

The above terms are input under format (4E12.4).

3. The second card has the following information:

Time	= actual time of test period (min.).	Col. 1-12
R	= number of temperature readings (always odd) $R < 100$.	Col. 13-24
TRO	= lowest reference temperature to be used (^oR).	Col. 25-36
TRF	= highest reference temperature to be used (^oR).	Col. 37-48
TRS	= size of step changes in reference temperatures used (^oR).	Col. 49-60

The input is under FORMAT (5F12.0), however, TRO, TRF, and TRS are treated as integer quantities.

4. The third card

   TNO = test description (name, number, etc.) Col. 1-20

   TNO is input under FORMAT (2A10).

5. The next series of cards contain one temperature reading per card (^{o}R), read in under FORMAT (F12.0) Col. 1-12

   There must be R cards in the series.

6. The above statements 4 and 5 may be repeated several times as a set.

Since the program ends with an error, a complete new set of data cards could be read in and used after the first set has been used. This would be accomplished by putting three more control cards in the deck to follow the normal "LGO" card. They should be the following:

```
EXIT.
.MODE O.
LGO.
```

A 7/8/9 card should separate the two sets of data.

The order in which the data cards are to be read in can easily be altered by relocating the read statements in the computer program. This shuffling of cards is possible since there are no statements directing a transfer to one of the read statements.

Example of such a READ statement switch.

If each set of temperatures were to be analyzed with respect to different reference temperatures or test times, one would switch the location of FORTRAN statements 1 and 4. In this case, the above INPUT description statement 6 would read "The above statements 3, 4, and 5 may be repeated several times as a set."

OUTPUT DATA

The program was written to print out the following information:

Actual test time (min.)

Equivalent corrosion time (min.)

Given reference temperature (°R)

List of input temperatures (°R)

A copy of the program and a sample of input and output data sheets follow.

```
RUN(S)
LGO.

      PROGRAM TIME(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
C     THIS PROGRAM IS TO DETERMINE AN EQUIVELENT CORROSION TIME AT A
C     PROPOSED TEMPERATURE.  INPUTING  A RATE OF REACTION OF MATERIAL
C     REMOVAL THE FOLLOWING PROGRAM WILL ATTEMPT TO SOLVE INTEGRAL
C     BY USE OF SIMPSONS METHOD.
C
C     KENNETH KOLBERG
C     THERMO FLOW LAB
C
C     INPUT = TEST NO.,NO. OF TEMP READINGS AT EQUAL INTERVALS,ACTUAL
C     TIME OF TEST, REFERENCE TEMP. RANGE, FOUR REACTION RATE CONSTANTS
C
      DIMENSION X(100),Y(100),T(100),TNO(2)
C
  100 FORMAT (2A10)
  101 FORMAT (4E12.4)
  102 FORMAT (5F12.0)
  103 FORMAT (F12.0)
  110 FORMAT(1H1///12X,25HEQUIVALENT CORROSION TIME////)
  111 FORMAT (12X,11HTEST NO. = ,2A10, /12X,13HACTUAL TIME =,F8.2/
     112X,17HREFERENCE TEMP. =,F6.0, 6H DEG.R/12X,17HREFERENCE TIME = ,
     2F8.2,5H MIN.///)
  112 FORMAT(15X,17HINPUT TEMPERATURE//)
  113 FORMAT(15X,F12.3)
C
    2 READ (5,101) A1,B1,A3,B3
    4 READ (5,102) TIME,R, TRO, TRF, TRS
    1 CONTINUE
    3 READ (5,100) TNO
      N = R
      KTRO = TRO
      KTRF = TRF
      KTRS = TRS
      DO 5 I = 1,N
      READ (5,103) T(I)
      X(I) = EXP(-B1/T(I))
    5 Y(I) = EXP(-B3/T(I))
C
C
      Z = A1*(X(1) + X(N)) + A3*(Y(1) + Y(N))
      M = N-1
      DO 10 I = 2,M,2
   10 Z = Z + 4.0*(A1*X(I)+ A3*Y(I))
C
```

```
      M = N-2
      DO 15 I = 3,M,2
   15 Z = Z + 2*(A1*X(I) + A3*Y(I))
C
      DO 20 J = KTRO,KTRF,KTRS
      REF = J
      C = A1 * EXP(-B1/REF) + A3 * EXP(-B3/REF)
      TREF = Z*TIME/(3.0 *(R-1.0)*C)
      WRITE (6,110)
      WRITE (6,111) TNO,TIME,REF,TREF
      WRITE (6,112)
      WRITE (6,113) (T(I),I=1,N)
   20 CONTINUE
      GO TO 1
      END
```

EGUIVALENT CORROSION TIME

TEST NO. = TEST NO. 1
ACTUAL TIME = 80.00
REFERENCE TEMP. = 3000 DEG.R
REFERENCE TIME = 522.37 MIN.

INPUT TEMPERATURE

530.000
2300.000
3220.000
3770.000
4040.000
3700.000
3610.000
3740.000
3760.000
3720.000
3760.000
3710.000
3650.000
3680.000
3720.000

EQUIVALENT CORROSION TIME

TEST NO. = TEST NO. 1
ACTUAL TIME = 80.00
REFERENCE TEMP. = 3500 DEG.R
REFERENCE TIME = 129.28 MIN.

INPUT TEMPERATURE

530.000
2300.000
3220.000
3770.000
4040.000
3700.000
3610.000
3740.000
3760.000
3720.000
3760.000
3710.000
3650.000
3680.000
3720.000

EGUIVALENT CORROSION TIME

TEST NO. = TEST NO. 1
ACTUAL TIME = 80.00
REFERENCE TEMP. = 4000 DEG.R
REFERENCE TIME = 35.91 MIN.

INPUT TEMPERATURE

530.000
2300.000
3220.000
3770.000
4040.000
3700.000
3610.000
3740.000
3760.000
3720.000
3760.000
3710.000
3650.000
3680.000
3720.000

FORM 33106 A

Westinghouse Electric Corporation

FORTRAN - CODING FORM

TITLE INPUT

ANAL	PHONE	DATE	PROGRAM NO.	DECK NO.	L.S. NO.

```
      1.00E-05   1.00E 04       0.20      4.00E 04
      80.        15.        3000.     4000.       500.
TEST NØ. 1
       530
      2300
      3220
      3770
      4040
      3700
      3610
      3740
      3760
      3720
      3760
      3710
      3650
      3680
      3720
```